

## **Quantum Lattice-Gas Representation of the Dirac Equation**

**Gerard T. Fairley**

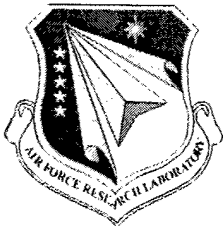
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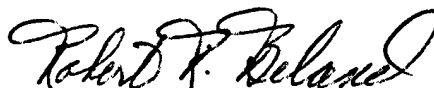
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This Technical Report has been reviewed and is approved for publication.



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13. ABSTRACT (Maximum 200 words)  This paper reports explicit quantum lattice-gas unitary matrix representations for the 1D and 2D Dirac equations, and the 1D, 2D, and 3D Weyl equations. It also clarifies some algorithms and results introduced in <i>Bialynicki-Birula</i> [1994] and <i>Meyer</i> [1996]. Most of the matrix solutions are well-suited for type-II quantum computers, such as NMR machines.				
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## 1. INTRODUCTION

Conventional classical supercomputers will likely reach their computational and/or feasible commercial cost limit in 20-30 years. It is extremely unlikely that many of the most difficult and important non-linear field theories like Navier-Stokes, QCD, General Relativity, and quantum gravity will be solved before these limits are realized. By far the most promising way forward appears to be through quantum computer development. It is also generally acknowledged that quantum computers will provide the most powerful system for simulations of quantum mechanics.

This paper develops primarily type-II quantum computer lattice-gas algorithms because of the apparently formidable unsolved technological obstacle of establishing completely globally phase-coherent type-I quantum computation. In particular the Weyl 1D, 2D, and 3D and Dirac 1D lattice-gas equations for relativistic quantum point particles are given.

Section two contains a derivation of the orthonormal properties of the  $W$  matrices. Section three discusses the lattice-gas algorithms of the 1D Weyl and Dirac equations in the context of the papers of [Bialynicki-Birula, I., 1994] and [Meyer, D. A., 1996]. Explicit lattice-gas algorithms, first order solutions, and implementations are presented for a specific representation. In section four an explicit first order lattice-gas solution of the 2D Weyl equation in a specific representation is presented. The exact two component spinor solution to the 2D Dirac equation is given. A numerically untested result and possible methods for obtaining the 2D Dirac lattice-gas solution is included. In section five an explicit first order lattice-gas solution to the 3D Weyl equation is presented in a specific representation.

## 2. ORTHOGONALITY AND UNITARITY CONDITIONS OF THE DISCRETE WEYL AND DIRAC PROPAGATOR

The Weyl equation describes the spinor of a rest-massless relativistic quantum point object while the Dirac equation describes the spinor of a massive relativistic quantum point object. For the Weyl solution, [Bialynicki-Birula, I., 1994] postulates a two component spinor  $\phi$  on a manifold with a body-centered 3D discrete Euclidean space lattice and a Newtonian time with the following Huygens-like propagation for each discrete update time  $\tau$ .  $W(\vec{h})$  is a 2x2 matrix operating at space point  $\vec{r} + \vec{h}$ ,

$$\phi(\vec{r}, t + \tau) = \sum_{\vec{h}} W(\vec{h}) \phi(\vec{r} + \vec{h}, t), \quad (1)$$

but for the Dirac solution  $W$  becomes a 4x4 matrix  $\tilde{D}$  and  $\phi$  becomes a four component spinor  $\tilde{\phi}$ <sup>1</sup>. Each of the members of the set of eight primitive lattice vectors  $\vec{h}$  start at  $\vec{r}$  and end at one of the eight corners of the cube defined by the first octant of the coordinate system originating at  $\vec{r}$ .

To determine the algebra of the 2x2  $W$  matrices first consider two equal-time independent spinors:

$$\begin{aligned} \phi(\vec{r}_1, t + \tau) &= \sum_{\vec{h}_1} W(\vec{h}_1) \phi(\vec{r}_1 + \vec{h}_1, t) \\ \phi^\dagger(\vec{r}_2, t + \tau) &= \sum_{\vec{h}_2} W^\dagger(\vec{h}_2) \phi^\dagger(\vec{r}_2 + \vec{h}_2, t). \end{aligned} \quad (2)$$

Now consider the overlap sum:

$$\sum_{\vec{r}_1, \vec{r}_2} \phi^\dagger(\vec{r}_2, t + \tau) \phi(\vec{r}_1, t + \tau) \delta_{\vec{r}_2 + \vec{h}_2, \vec{r}_1 + \vec{h}_1} \quad (3)$$

Thus for set elements satisfying  $\vec{h} \neq \vec{h}'$  the above Kronecker delta function allows the product of partially overlapping ( $\vec{r}_1 \neq \vec{r}_2$ ) spinors to be non-trivial. But we will demand, as

<sup>1</sup>All tilded operators following are 4x4 matrices and non-tilded matrices are 2x2.

Bialynicki-Birula did, that the sum of these products is trivial. The Kronecker delta also defines a maximum separation for non-trivial overlap that occurs when  $\vec{h} = -\vec{h}'$ , e.g. at opposite corners of the first octant. Equivalently, and using Eq. (2):

$$\sum_{\vec{r}_1, \vec{r}_2} \phi^\dagger(\vec{r}_2, t + \tau) \phi(\vec{r}_1, t + \tau) \delta_{\vec{r}_2, \vec{r}_1 + \vec{h} - \vec{h}'} = \sum_{\vec{h}_1, \vec{h}_2, \vec{r}_1, \vec{r}_2} W^\dagger(\vec{h}_2) W(\vec{h}_1) \phi^\dagger(\vec{r}_2 + \vec{h}_2, t) \phi(\vec{r}_1 + \vec{h}_1, t) \delta_{\vec{r}_2, \vec{r}_1 + \vec{h} - \vec{h}'}. \quad (4)$$

Hence:

$$\sum_{\vec{r}_1} \phi^\dagger(\vec{r}_1 + \vec{h} - \vec{h}', t + \tau) \phi(\vec{r}_1, t + \tau) = \sum_{\vec{h}_1, \vec{h}_2, \vec{r}_1} W^\dagger(\vec{h}_2) W(\vec{h}_1) \phi^\dagger(\vec{r}_1 + \vec{h} - \vec{h}' + \vec{h}_2, t) \phi(\vec{r}_1 + \vec{h}_1, t). \quad (5)$$

The normalization condition,

$$\sum_{\vec{r}} \phi^\dagger(\vec{r}, t) \phi(\vec{r}, t) = 1 \quad (6)$$

can be re-written for the new time  $t + \tau$  as

$$\sum_{\vec{r}_1} \phi^\dagger(\vec{r}_1 + \vec{h} - \vec{h}', t + \tau) \phi(\vec{r}_1, t + \tau) = \delta_{\vec{h} - \vec{h}', 0} \quad (7)$$

and hence:

$$\sum_{\vec{r}_1} \phi^\dagger(\vec{r}_1 + \vec{h} - \vec{h}' + \vec{h}_2, t) \phi(\vec{r}_1 + \vec{h}_1, t) = \delta_{\vec{h} - \vec{h}' + \vec{h}_2, \vec{h}_1}. \quad (8)$$

Thus, we have equivalently from Eqs. (5), (7), and (8) the orthonormal conditions for the  $W$  matrices:

$$\delta_{\vec{h} - \vec{h}', 0} = \sum_{\vec{h}_1, \vec{h}_2} W^\dagger(\vec{h}_2) W(\vec{h}_1) \delta_{\vec{h} - \vec{h}' + \vec{h}_2, \vec{h}_1}. \quad (9)$$

And equivalently the orthonormal conditions are more simply:

$$\delta_{\vec{h} - \vec{h}', 0} = \sum_{\vec{h}_1} W^\dagger(\vec{h}_1 + \vec{h}' - \vec{h}) W(\vec{h}_1). \quad (10)$$

### 3. THE ONE-DIMENSIONAL WEYL AND DIRAC EQUATIONS

Bialynicki-Birula's 1D Weyl algorithm and Meyer's 1D Dirac algorithm [Meyer, D. A., 1996], e.g. Eq. (1), both have the same implicit form,

$$\phi(x, t + \tau) = W(-h)\phi(x - h, t) + W(h)\phi(x + h, t) \quad (11)$$

but the explicit matrix elements are different. Though it is not by design, Meyer's matrices (equation (17) of [Meyer, D. A., 1996]) substituted for Bialynicki-Birula's 1D matrices reproduces the required orthonormality and Bialynicki-Birula's helicity relation,

$$W(-\vec{h}) = \sigma_y W^*(\vec{h}) \sigma_y. \quad (12)$$

The Bialynicki-Birula 1D algorithm (see Eqs. (39) and (40) of [Bialynicki-Birula, I., 1994]), for the Dirac equation yields the same correct result as Meyer's because the four-spinor difference update equations decouple into two independent particle and anti-particle two-component spinor update equations, each equivalent to Meyer's result. Writing  $\phi = \begin{pmatrix} \phi_L \\ \phi_R \end{pmatrix}$ , expanding and collecting components the difference update equations are:

$$\begin{pmatrix} \phi_L(x, t + \tau) \\ \phi_R(x, t + \tau) \end{pmatrix} = \begin{pmatrix} \cos(\theta) & i\sin(\theta) \\ i\sin(\theta) & \cos(\theta) \end{pmatrix} \begin{pmatrix} \phi_L(x + h, t) \\ \phi_R(x - h, t) \end{pmatrix} \quad (13)$$

Now by using a streaming operator  $S_x$ ,

$$S_x \begin{pmatrix} \phi_L(x, t) \\ \phi_R(x, t) \end{pmatrix} \equiv \begin{pmatrix} \phi_L(x + h, t) \\ \phi_R(x - h, t) \end{pmatrix} \quad (14)$$

one can re-write the lattice-gas equation (13) as:

$$\begin{pmatrix} \phi_L(x, t + \tau) \\ \phi_R(x, t + \tau) \end{pmatrix} = \begin{pmatrix} C & S_x \end{pmatrix} \begin{pmatrix} \phi_L(x, t) \\ \phi_R(x, t) \end{pmatrix} \quad (15)$$

with  $C$  given by the collision operator shown in (13) above. Using Mathematica [Wolfram, S., 2001] this lattice-gas algorithm can be implemented using symbolic terms which can then be expanded in terms of the lattice spacing. The following symbolic psuedo-code difference scheme has lattice period  $\tau = 2$  and the amplitudes  $\phi$  are initialized at time  $t=0$ :

```
if mod[n,2] = 0;
     $\phi_L[l, n] = \cos(\theta)\phi_L[l, n - 1] + i\sin(\theta)\phi_R[l, n - 1];$ 
```



```

 $\phi_R[l, n] = i \sin(\theta) \phi_L[l, n - 1] + \cos(\theta) \phi_R[l, n - 1];$ 
if mod[n,2] = 1;
 $\phi_L[l, n] = \phi_L[l + 1, n - 1];$ 
 $\phi_R[l, n] = \phi_R[l - 1, n - 1];$ 
do l,1,numberofgridpoints
 $\phi_L[l, 0] = \text{phiL}[l];$ 
 $\phi_R[l, 0] = \text{phiR}[l];$ 
end do

```

Once the above has been executed, the Mathematica [Wolfram, S., 2001] command

$$\text{Table}[\{\phi_L[l, n], \phi_R[l, n]\}, \{t, 0, 2\}], \quad (16)$$

or some equivalent form of Do loop then produces the values of  $\phi$  for all the integer  $t$  values. These terms then must be expanded to first order in the lattice spacing using fourier series (see equation (24) for an example).

For  $\theta = 0$  Bialynicki-Birula's Weyl equation algorithm is recovered and to first order in the lattice spacing  $\delta x$  (e.g. use approximations like  $\phi_L[l - 1, 0] = \phi_L[l, 0] + \delta x \phi_L^{(1,0)}[l, 0]$ ), this reproduces the 1D massless Weyl equation. Bialynicki-Birula's 1D Weyl matrices can be explicitly found from linear combinations of his P matrices:  $W(h) = (P_1 + P_3)/2$  and  $W(-h) = (P_2 - P_4)/2$ . For the case  $\theta = m\epsilon$  where  $\epsilon$  is an infinitesimal scalar the 1D massive Dirac equation results to first order in both  $\epsilon$  and the lattice spacing. This is, of course, what Feynman proved [Feynman, R. P. and Hibbs, A. R., 1965]. And, as required, the Weyl equation results for  $m=0$  and this is mathematically equivalent to the case  $\theta = 0$ . Although there appeared no recognizable symbolic result for a finite and non-trivial  $\theta$  Meyer gives some results [Meyer, D. A., 1996] connecting non-trivial finite  $\theta$  values with finite velocity propagation.

The Weyl equation and the Dirac equation can thus be modeled with the same algorithm but the Weyl model requires all finite matrix parameter values and the Dirac model requires some infinitesimal matrix parameter values. Bialynicki-Birula's stated algorithms for the 1D Weyl and Dirac equations are correct. Since it is not exactly clear how to interpret the Dirac algorithm using non-infinitesimal  $\theta$  values one must choose some  $\epsilon$  magnitude that is sufficiently small for the precision required to reproduce the behavior of a Dirac object. Bialynicki-Birula's 2D and 3D algorithms behave similarly.

One can derive the 1D and 2D Dirac differential equations and the 1D, 2D, and 3D Weyl

differential equations by considering Dirac's equation

$$i\hbar\partial_t\psi = \frac{\hbar c}{i}\alpha \cdot \nabla\psi + mc^2\beta\psi \quad (17)$$

where  $\alpha$  and  $\beta$  are each replaced by one of the 2x2 Pauli matrices  $\vec{\sigma}$  and  $m=0$  for the Weyl equation. Thus there are six possible representations, or equations, for the 1D Dirac equation and three possible representations for the 1D Weyl equation. The 'square' of each equation yields a Klein-Gordon equation. Only for the massive case in three space dimensions are 4x4 matrices required for equation (17). [Jacobson, T. and Shulman, L. S., 1984] take  $\alpha = \sigma_z$  and  $\beta = -\sigma_x$  which gives

$$\begin{aligned} i\hbar\partial_t\psi_1 &= \frac{\hbar c}{i}\partial_x\psi_1 - mc^2\psi_2 \\ i\hbar\partial_t\psi_2 &= -\frac{\hbar c}{i}\partial_x\psi_2 - mc^2\psi_1 \end{aligned} \quad (18)$$

These equations are solved to first order in both the lattice spacing and in  $\epsilon$  by the lattice-gas algorithm (15) and

$$C = \begin{pmatrix} \cos(m\epsilon) & i\sin(m\epsilon) \\ i\sin(m\epsilon) & \cos(m\epsilon) \end{pmatrix}. \quad (19)$$

#### 4. THE TWO-DIMENSIONAL WEYL AND DIRAC EQUATIONS

As with Bialynicki-Birula we choose  $W_i = 1/2 P_i$  so the 2D W matrices are

$$\begin{aligned} W_1 &= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad W_2 = \frac{1}{2} \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \\ W_3 &= \frac{1}{2} \begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \quad W_4 = \frac{1}{2} \begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}. \end{aligned} \quad (20)$$

The 2D Weyl differential equation is obtained from Dirac's equation, (17), with  $m=0$ :

$$i\hbar \partial_t \psi = \frac{\hbar c}{i} (\alpha_x \partial_x \psi + \alpha_y \partial_y \psi). \quad (21)$$

There are six possible representations, or equations, depending on which components of  $\vec{\sigma}$  are substituted for which of  $\alpha_x$  and  $\alpha_y$ . One possible choice  $\alpha_x = \sigma_z$ ,  $\alpha_y = \sigma_x$ , gives the explicit equation

$$\begin{aligned} \partial_t \psi_1 &= c(-\partial_x \psi_1 - \partial_y \psi_2) \\ \partial_t \psi_2 &= c(+\partial_x \psi_2 - \partial_y \psi_1). \end{aligned} \quad (22)$$

The following unitary lattice-gas algorithm reproduces this representation of the 2D Weyl equation to first order in lattice spacing:

$$\begin{pmatrix} \phi_L(x, y, t + \tau) \\ \phi_R(x, y, t + \tau) \end{pmatrix} = \begin{pmatrix} C_b & S_y & C_a & S_x \end{pmatrix} \begin{pmatrix} \phi_L(x, y, t) \\ \phi_R(x, y, t) \end{pmatrix}. \quad (23)$$

The explicit result after one period  $\tau$  is given, using Mathematica [Wolfram, S., 2001], by

$$i(\phi_L[l, m, \tau] - \phi_L[l, m, 0])/\epsilon = -i\delta s(\phi_R^{(0,1,0)}[l, m, 0] + \phi_L^{(1,0,0)}[l, m, 0])/\epsilon, \quad (24)$$

where  $S_x$  and  $S_y$  act as the streaming operator  $S$  from before but now act only on the indicated variable. The  $C$  matrices were determined algebraically by expanding out the

difference equation (21) and equating the corresponding matrix elements of relation (1) substituted with the above 2D W matrices in (20):

$$C_a = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} \text{ and } C_b = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}. \quad (25)$$

Then the helicity relation (12) yields

$W(\vec{h})$	$W(-\vec{h})$
$W_1$	$W_4$
$W_2$	$W_3$
$W_3$	$W_2$
$W_4$	$W_1$

Substitution of these  $2 \times 2$  W matrices into equations (39) and (40) of [Bialynicki-Birula, I. 1994] gives a four component difference equation for the 2D Dirac equation.

The 2D Dirac equation is obtained from Eq. (17):

$$i\hbar\partial_t\psi = \frac{\hbar c}{i}(\alpha_x\partial_x\psi + \alpha_y\partial_y\psi) + \beta mc^2\psi. \quad (26)$$

There are  $3!$  possible representations, or equations, depending on which components of  $\vec{\sigma}$  are substituted for which of  $\alpha_x$ ,  $\alpha_y$  and  $\beta$ . One possible choice  $\alpha_x = \sigma_x$ ,  $\alpha_y = \sigma_y$ , and  $\beta = \sigma_z$  gives the explicit equation

$$\begin{aligned} i\hbar\partial_t\psi_1 &= \frac{\hbar c}{i}(\partial_x\psi_2 - i\partial_y\psi_2) + mc^2\psi_1 \\ i\hbar\partial_t\psi_2 &= \frac{\hbar c}{i}(\partial_x\psi_1 + i\partial_y\psi_1) - mc^2\psi_2. \end{aligned} \quad (27)$$

The formal solution to Eq. (26) is obtained by determination of S for

$$\psi'(x', y', t') = S\psi(x, y, t), \quad (28)$$

with the result:

$$S = \sqrt{\frac{E + mc^2}{2mc}} \begin{pmatrix} 1 & \frac{p-c}{E+mc^2} \\ \frac{p+c}{E+mc^2} & 1 \end{pmatrix}. \quad (29)$$

Bialynicki-Birula's 4x4  $\tilde{D}$  matrices for

$$\tilde{\phi}(\vec{r}, t + \tau) = \sum_{\vec{h}} \tilde{D}(\vec{h}) \tilde{\phi}(\vec{r} + \vec{h}, t) \quad (30)$$

are explicitly represented by:

$$\begin{aligned} \tilde{D}_1 &= \frac{1}{2} \begin{pmatrix} \cos(m\epsilon) & 0 & 0 & -i\sin(m\epsilon) \\ \cos(m\epsilon) & 0 & 0 & i\sin(m\epsilon) \\ i\sin(m\epsilon) & 0 & 0 & -\cos(m\epsilon) \\ i\sin(m\epsilon) & 0 & 0 & \cos(m\epsilon) \end{pmatrix}, \quad \tilde{D}_2 = \frac{1}{2} \begin{pmatrix} 0 & \cos(m\epsilon) & i\sin(m\epsilon) & 0 \\ 0 & \cos(m\epsilon) & -i\sin(m\epsilon) & 0 \\ 0 & i\sin(m\epsilon) & \cos(m\epsilon) & 0 \\ 0 & i\sin(m\epsilon) & -\cos(m\epsilon) & 0 \end{pmatrix}, \\ \tilde{D}_3 &= \frac{1}{2} \begin{pmatrix} \cos(m\epsilon) & 0 & 0 & i\sin(m\epsilon) \\ -\cos(m\epsilon) & 0 & 0 & i\sin(m\epsilon) \\ i\sin(m\epsilon) & 0 & 0 & \cos(m\epsilon) \\ -i\sin(m\epsilon) & 0 & 0 & \cos(m\epsilon) \end{pmatrix}, \quad \tilde{D}_4 = \frac{1}{2} \begin{pmatrix} 0 & -\cos(m\epsilon) & i\sin(m\epsilon) & 0 \\ 0 & \cos(m\epsilon) & i\sin(m\epsilon) & 0 \\ 0 & -i\sin(m\epsilon) & \cos(m\epsilon) & 0 \\ 0 & i\sin(m\epsilon) & \cos(m\epsilon) & 0 \end{pmatrix}. \end{aligned} \quad (31)$$

Since Bialynicki-Birula's difference equation for the 2D Dirac equation uses four-component spinors but the solution of the 2D Dirac equation mathematically only necessitates two-component spinors, a lattice-gas equation explicitly equivalent to Eq. (23) was postulated, again with 2x2 matrices, and these coefficients were equated to the coefficients of some two-component subset of Bialynicki-Birula's four-component spinor equation. The exact form of a free four-component Dirac spinor in 2D was solved and used as a guideline for choosing the spinor components. Here are the positive and negative energy spinors in the rest frame at  $t=0$ :

Positive energy

$$\tilde{\omega}^1(\vec{p}) = \sqrt{\frac{E + mc^2}{2mc^2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \frac{p+c}{E+mc^2} \end{pmatrix}, \quad \tilde{\omega}^2(\vec{p}) = \sqrt{\frac{E + mc^2}{2mc^2}} \begin{pmatrix} 0 \\ 1 \\ \frac{p-c}{E+mc^2} \\ 0 \end{pmatrix} \quad (32)$$

Negative energy

$$\tilde{\omega}^3(\vec{p}) = \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} 0 \\ \frac{p+c}{E+mc^2} \\ 1 \\ 0 \end{pmatrix}, \quad \tilde{\omega}^4(\vec{p}) = \sqrt{\frac{E+mc^2}{2mc^2}} \begin{pmatrix} \frac{p-c}{E+mc^2} \\ 0 \\ 0 \\ 1 \end{pmatrix} \quad (33)$$

It is interesting that for infinitesimal  $\theta$  values the elements of the rows of Bialynicki-Birula's  $\tilde{D}$  matrices have a similarity to the large and small magnitude elements of the fundamental orthonormal Dirac spinors in the above shown 'large and small' representation and in the case of the null lightcone surface  $p_\mu x^\mu = 0$ . The resulting equations are inconsistent. Thus to obtain the lattice-gas representation of the 2D Dirac equation using 2x2 matrices one has to either guess, derive the explicit form of the 2x2 propagator solutions as Feynman[Schweber, S. S., 1986] attempted (and remains currently unsolved), or try to "reverse engineer" Bialynicki-Birula's non-unitary four component spinor difference equation. Doing the latter did yield some unitary results. The lattice-gas equation obtained is:

$$\tilde{U}\tilde{\phi}(x, y, t) = \tilde{\phi}(x, y, t + \tau), \quad (34)$$

where  $\tilde{U}$  is a 4x4 matrix and

$$\tilde{U} = (\tilde{S}_x \tilde{O}_1 \tilde{S}_y + \tilde{G} \tilde{S}_x \tilde{O}_2 \tilde{S}_y + \tilde{S}_x \tilde{O}_3 \tilde{S}_y \tilde{G} + \tilde{G} \tilde{S}_x \tilde{O}_4 \tilde{S}_y \tilde{G}) \tilde{S}_0 \quad (35)$$

with

$$\begin{aligned} \tilde{O}_1 &= \begin{pmatrix} (A_1 + A_2)/2 & -(D_1 + D_2)/2 \\ (C_1 - C_2)/2 & (B_1 - B_2)/2 \end{pmatrix}, \quad \tilde{O}_2 = \begin{pmatrix} (A_1 + A_2)/2 & (D_1 + D_2)/2 \\ (C_1 - C_2)/2 & -(B_1 - B_2)/2 \end{pmatrix}, \\ \tilde{O}_3 &= \begin{pmatrix} (B_1 + B_2)/2 & (C_1 + C_2)/2 \\ -(D_1 - D_2)/2 & (A_1 - A_2)/2 \end{pmatrix}, \quad \tilde{O}_4 = \begin{pmatrix} -(B_1 + B_2)/2 & (C_1 + C_2)/2 \\ (D_1 - D_2)/2 & (A_1 - A_2)/2 \end{pmatrix}, \end{aligned} \quad (36)$$

and,

$$\tilde{S}_x = \begin{pmatrix} S_x & 0 \\ 0 & S_x \end{pmatrix}, \quad \tilde{S}_y = \begin{pmatrix} S_y & 0 \\ 0 & S_y \end{pmatrix}, \quad \tilde{S}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad (37)$$

and,

$$\tilde{G} = \begin{pmatrix} G & 0 \\ 0 & G \end{pmatrix}, \quad \text{with } G = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad (38)$$

and,

$$\begin{aligned}
A_1 &= \begin{pmatrix} \cos(m\epsilon) & i\sin(m\epsilon) \\ i\sin(m\epsilon) & \cos(m\epsilon) \end{pmatrix}, \quad A_2 = \begin{pmatrix} \cos(m\epsilon) & i\sin(m\epsilon) \\ -i\sin(m\epsilon) & -\cos(m\epsilon) \end{pmatrix}, \\
B_1 &= \begin{pmatrix} -i\sin(m\epsilon) & \cos(m\epsilon) \\ -\cos(m\epsilon) & i\sin(m\epsilon) \end{pmatrix}, \quad B_2 = \begin{pmatrix} -i\sin(m\epsilon) & \cos(m\epsilon) \\ \cos(m\epsilon) & -i\sin(m\epsilon) \end{pmatrix}, \\
C_1 &= \begin{pmatrix} i\sin(m\epsilon) & \cos(m\epsilon) \\ \cos(m\epsilon) & i\sin(m\epsilon) \end{pmatrix}, \quad C_2 = \begin{pmatrix} -i\sin(m\epsilon) & -\cos(m\epsilon) \\ \cos(m\epsilon) & i\sin(m\epsilon) \end{pmatrix}, \\
D_1 &= \begin{pmatrix} \cos(m\epsilon) & -i\sin(m\epsilon) \\ i\sin(m\epsilon) & -\cos(m\epsilon) \end{pmatrix}, \quad D_2 = \begin{pmatrix} -\cos(m\epsilon) & i\sin(m\epsilon) \\ i\sin(m\epsilon) & -\cos(m\epsilon) \end{pmatrix},
\end{aligned} \tag{39}$$

with  $G$  a swap matrix for a two-component spinor, and  $S_x$  and  $S_y$  are the usual streaming operators that act on two-component spinors. All component matrices of  $\tilde{U}$  are unitary. Since the streaming operators do not have explicit form in this representation the following assignments develop the unitarity of  $\tilde{U}$ .

The following operator equalities are found to hold:

$$\begin{aligned}
\tilde{O}_2^\dagger O_4 &= -\tilde{O}_1^\dagger O_3 \\
O_3 \tilde{O}_4^\dagger &= -O_1 \tilde{O}_2^\dagger.
\end{aligned} \tag{40}$$

By considering terms from  $\tilde{U}^\dagger \tilde{U} = 1$ , we are led to determine the constants  $a$  and  $b$  in:

$$\begin{aligned}
\tilde{O}_2^\dagger O_4 &= -\tilde{O}_1^\dagger O_3 \equiv a \tilde{S}_y \tilde{G} \tilde{S}_y^\dagger \\
O_3 \tilde{O}_4^\dagger &= -O_1 \tilde{O}_2^\dagger \equiv b \tilde{S}_x \tilde{G} \tilde{S}_x^\dagger.
\end{aligned} \tag{41}$$

Using Eq. (41) in  $\tilde{U}$  gives the following terms,

$$\begin{aligned}
\tilde{G} \tilde{S}_x \tilde{O}_2 \tilde{S}_y &= -\frac{1}{b} \tilde{S}_x \tilde{O}_1 \tilde{S}_y \\
\tilde{S}_x \tilde{O}_3 \tilde{S}_y \tilde{G} &= -\frac{1}{a} \tilde{S}_x \tilde{O}_3 \tilde{O}_1^\dagger \tilde{O}_3 \tilde{S}_y \\
\tilde{G} \tilde{S}_x \tilde{O}_4 \tilde{S}_y \tilde{G} &= -\frac{1}{ab} \tilde{S}_x \tilde{O}_3 \tilde{O}_1^\dagger \tilde{O}_3 \tilde{S}_y,
\end{aligned} \tag{42}$$

which when substituted into  $\tilde{U}$  gives, with  $a=2$  and  $b=1$ :

$$\begin{aligned}\tilde{U} &= -\tilde{S}_x \tilde{O}_p \tilde{S}_y \tilde{S}_0 \\ \tilde{O}_p &= \tilde{O}_3 \tilde{O}_1^\dagger \tilde{O}_3.\end{aligned}\tag{43}$$

This  $\tilde{U}$  is unitary and is thus suitable for type-II quantum computers.



## 5. THE THREE-DIMENSIONAL WEYL AND DIRAC EQUATIONS

The 3D Weyl differential equation is obtained from Dirac's equation, (17), with  $m=0$ :

$$i\hbar\partial_t\psi = \frac{\hbar c}{i}\alpha \cdot \nabla\psi \quad (44)$$

There are 3! possible representations, or equations, depending on which components of  $\vec{\sigma}$  are substituted for which components of  $\vec{\alpha}$ . One possible choice  $\alpha_x = \sigma_z$ ,  $\alpha_y = \sigma_x$ , and  $\alpha_z = \sigma_y$  gives the explicit equation

$$\begin{aligned} \partial_t\psi_1 &= c(-\partial_x\psi_1 - \partial_y\psi_2 + i\partial_z\psi_2) \\ \partial_t\psi_2 &= c(+\partial_x\psi_2 - \partial_y\psi_1 - i\partial_z\psi_1). \end{aligned} \quad (45)$$

The following unitary lattice-gas algorithm reproduces this 3D Weyl equation to first order in lattice spacing:

$$\begin{pmatrix} \phi_L(x, y, z, t + \tau) \\ \phi_R(x, y, z, t + \tau) \end{pmatrix} = \begin{pmatrix} C_3 & S_z & C_2 & S_y & C_1 & S_x \end{pmatrix} \begin{pmatrix} \phi_L(x, y, z, t) \\ \phi_R(x, y, z, t) \end{pmatrix} \quad (46)$$

where  $S_x$ ,  $S_y$ , and  $S_z$  act as the streaming operators. The  $C$  matrices are determined algebraically by expanding the two component spinor difference equation (46) and equating the corresponding matrix elements of equation (1) substituted with the 2x2  $W$  matrices given in Eq. (12) of [Bialynicki-Birula, I., 1994]. These  $W$ 's are simple multiples of the 2D  $W$ 's used above. Three equivalent matrices are then:

$$C_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} -\exp(i\pi/4) & -\exp(i\pi/4) \\ \exp(-i\pi/4) & -\exp(-i\pi/4) \end{pmatrix}, \text{ and } \tilde{C}_3 = \tilde{C}_2 = \tilde{C}_1. \quad (47)$$

Equation (46) solves our particular representation, (45), of the 3D Weyl equation. The lattice-gas solutions to the 3D Dirac equation may emerge from algebraic comparison similar to one of those stated above. The  $W$  matrices required are supplied in Bialynicki-Birula and four component spinor lattice-gas matrices may be required.



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